

# Relativistic coupled cluster calculations of spectroscopic and chemical properties for element 120

L.V. Skripnikov,<sup>1,\*</sup> N.S. Mosyagin,<sup>1</sup> and A.V. Titov<sup>1</sup>

<sup>1</sup>*Federal state budgetary institution "Petersburg Nuclear Physics Institute", Gatchina, Leningrad district 188300, Russia*

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The coupled cluster calculations with accounting for relativistic effects to study spectroscopic and chemical properties of element 120 (E120) are performed. Similar calculations for Ba are also done and they are in a good agreement with the experimental data. Dissociation energies of diatomic X-H and X-Au molecules, where X=E120, Ba, are calculated; for E120 they are found to be  $1.5 \div 2$  times smaller than those for Ba.

## INTRODUCTION

At present all the relatively long-lived superheavy elements (SHEs) up to the seventh period of the Periodic table were synthesized in FLNR JINR (see [1, 2] and references) and their synthesis was mainly confirmed in LBNL [3] and GSI [4]. The new challenge for nuclear physics is the synthesis of the elements of the eight period.

According to its position in the Periodic table, element 120 (E120) is supposed to be the  $s$  element and homologue of Ba and Ra. The earlier obtained ground state configuration of E120 at the Dirac-Fock level,  $7s^2 7p^6 8s^2$ , is confirmed in recent calculation [5] using the correlation potential method. Relativistic stabilization of the valence  $s$  orbital [6, 7] leads in general to higher excitation energies from this shell and, as a consequence, to weakening the bond strengths in its chemical compounds. Therefore, E120 can resemble the noble gas rather than to the alkaline earth element. Provided that E120 is synthesized, its properties can be investigated experimentally by the gas-phase chromatography method. Such scheme was successfully employed in FLNR JINR [8] and GSI [4] for E112 and E114 where gold served as adsorbent. Theoretical calculations are required for planning similar experiments with E120 on the gold surface.

We have performed calculations of excitation energies of the E120 atom and its cation,  $E120^+$ , as well as of spectroscopic properties of the E120H and E120Au molecules compared to the analogous systems with Ba, for which some experimental data are available.

## CALCULATION METHOD

To calculate properties of E120, the generalized relativistic effective core potential (GRECP) method [9] was employed. For relativistic correlation calculations, the fully-relativistic Fock-space coupled cluster code with single and double cluster amplitudes (FS-RCCSD) [7, 10] was applied. To calculate corrections on enlargement of the basis set and higher cluster amplitudes, the CFOUR [11] and MRCC [12, 13] codes were used.

## GRECP generation and atomic calculations

The GRECP for E120 was generated in the framework of the present work. To check performance of the GRECP method for such a heavy element, relativistic correlation calculations on the E120 atom and its cations were carried out. We used four-component calculations with Dirac-Coulomb-Breit (DCB) Hamiltonian and Fermi nuclear charge distribution ( $A = 304$ ) as the reference calculations. This Hamiltonian takes into account the great bulk of the relativistic effects including the relativistic corrections to the Coulomb interaction between electrons. The  $1-5s$ ,  $2-5p$ ,  $3-5d$ , and  $4-5f$  shells were frozen from the ground state  $E120^{2+}$  calculation. The 28 electrons (occupying the  $6spd, 7spd, 8sp$  shells) were correlated in the  $[12, 14, 14, 13, 12, 11]$  basis set of  $6-17s_{1/2}$ ,  $6-19p_{1/2}$ ,  $6-19p_{3/2}$ ,  $\dots$   $6-16h_{11/2}$  numerical spinors localized in the same radial space region as the  $6spd, 7spd, 8sp$  spinors. The correlations were taken into account with the help of the FS-RCCSD method. The closed-shell ground state of  $E120^{2+}$  was the reference state and the Fock-space scheme was

$$E120^{2+} \rightarrow E120^+ \rightarrow E120, \quad (1)$$

with electrons added to the  $8s_{1/2}$ ,  $8p_{1/2}$ ,  $8p_{3/2}$ ,  $7d_{3/2}$ , and  $7d_{5/2}$  spinors (the relativistic configurations corresponding to the nonrelativistic  $8p^2$ ,  $7d^2$ , and  $8p^1 7d^1$  ones were excluded from the model space).

The leading configurations and terms for the lowest-lying states of the E120 atom and its cations are presented in the first and second columns of table I. The results of the semiempirically-fitted CI/MBPT calculations with Dirac-Coulomb Hamiltonian [5, 14] are compared with our FS-RCCSD results in the third and fourth columns. They are in a reasonable agreement. The absolute errors due to decrease in the number of the correlated electrons, the neglect of a finite nuclear size or Breit interactions are listed in the last four columns. One can see that a finite nuclear size should be taken into account, whereas the correlations with the  $6spd$  electrons and Breit interactions can be neglected for the accuracy within  $2\text{ kcal/mol} \approx 700\text{ cm}^{-1}$  for one-electron excitations.

We have generated the GRECP for only 10 explicitly

TABLE I: Transition energies (TE) from DCB/FS-RCCSD calculations of the lowest-lying states of the E120 atom and its cations for 28 correlated electrons with Fermi nuclear model and Breit interactions taken into account. Absolute errors of reproducing the TE in the different versions of the four-component calculations. All values are in  $\text{cm}^{-1}$ .

Number of corr.el.:		28		20		10		28	
		TE		TE		TE		TE	
		Ref.		Abs.errors		Point without		Breit	
Leading conf.	Term	[5, 14]				nucl.			
$8s_{1/2}^1$	(J=1/2) $\rightarrow$								
$8p_{1/2}^1$	(J=1/2)	24851	24551	55	-372	1299		-51	
$7d_{3/2}^1$	(J=3/2)		25355	43	-151	1714		135	
$7d_{5/2}^1$	(J=5/2)		27529	20	-481	1661		152	
$8p_{3/2}^1$	(J=3/2)	38057	37643	23	-401	1632		62	
$E120^{2+}$	(J=0)	89931	89601	36	-620	1592		77	
$8s_{1/2}^2$	(J=0) $\rightarrow$								
$8s_{1/2}^1 8p_{1/2}^1$	(J=0)	16061	15328	58	-290	975		-45	
$8s_{1/2}^1 8p_{1/2}^1$	(J=1)	17968	17382	50	-290	1015		-30	
$8s_{1/2}^1 7d_{3/2}^1$	(J=1)	23066	22337	30	-145	1242		101	
$8s_{1/2}^1 7d_{3/2}^1$	(J=2)	23231	22494	24	-249	1212		101	
$8s_{1/2}^1 7d_{5/2}^1$	(J=3)	23827	23377	12	-418	1186		108	
$8s_{1/2}^1 8p_{3/2}^1$	(J=2)	25457	25308	26	-264	1186		42	
$8s_{1/2}^1 7d_{5/2}^1$	(J=2)	27477	27652	15	-401	1347		100	
$8s_{1/2}^1 8p_{3/2}^1$	(J=1)	27685	28304	3	-422	1024		39	
$8s_{1/2}^1$	(J=1/2)	47296	47633	11	-458	906		40	

treated electrons of E120 (i.e. with the  $7spd, 8sp, 6f, 5g$  GRECP components) following the scheme [15] just to reduce unnecessary computational efforts at the stage of correlation molecular calculations (see below); similar GRECP version was generated earlier for Ba [16]. The results for 10 correlated electrons (occupying the  $7spd, 8sp$  shells) in the [9,11,11,9,8,7] basis set of  $7-15s_{1/2}, 7-17p_{1/2}, 7-17p_{3/2}, \dots 6-12h_{11/2}$  numerical spinors localized in the same radial space region as the  $7spd, 8sp$  spinors are presented in table II. Transition energies from the DCB/FS-RCCSD calculations with Fermi nuclear model and the absolute errors of their reproducing in the GRECP calculations are tabulated in the third and fourth columns.

Different approximations to the “full” GRECP calculations are considered in the last four columns. If one neglects the difference between the outercore ( $7sp$ ) and valence ( $8sp$ ) GRECP components, two extreme GRECP versions can be derived with the conventional semi-local RECP operator: only valence or only outercore GRECP components acting on both the valence and outercore electrons. These cases are referred to as the valence or core GRECP versions, respectively [9]. One can see that the full and valence GRECP versions are suitable for the accuracy of  $2 \text{ kcal/mol} \approx 700 \text{ cm}^{-1}$  whereas the core GRECP version is not. It should be noted that the errors of neglecting the innercore correlations with the  $6spd$  shells and the errors of the GRECP approximation are partly compensating each other, thus, it additionally jus-

tifies our choice of the 10-electron GRECP for the present molecular calculations.

The scalar-relativistic (SR) calculations, i.e. without spin-orbit (SO) part of the valence GRECP operator, are presented in the seventh column. The SO contributions are large and should be taken into account. The scalar-relativistic SCF calculations followed by the FS-RCCSD calculations with the SO part of the valence GRECP operator are presented in the last column. These errors are comparable with the errors of the valence GRECP calculations in the fifth column. It should be emphasized that the GRECP calculations in the 4–6-th columns were carried out with the SO part at both the SCF and FS-RCCSD stages. The computational versions used in the last two columns (the SR SCF calculation followed by the scalar-relativistic or fully-relativistic coupled cluster study) are also used in the molecular correlation calculations discussed below.

TABLE II: Transition energies (TE) from DCB/FS-RCCSD calculations of the lowest-lying states of the E120 atom and its cations for 10 correlated electrons with Fermi nuclear model and Breit interaction are taken into account. Absolute errors of reproducing the TE with different versions of the GRECP calculations. All values are in  $\text{cm}^{-1}$ .

		TE		GRECP abs.errors		val.	
Leading conf.	Term	DCB	full	val.	core	val. SR-SCF	val. SO-RCC
$8s_{1/2}^1$	(J=1/2) $\rightarrow$						
$8p_{1/2}^1$	(J=1/2)	24142	247	306	-2761	9255	393
$7d_{3/2}^1$	(J=3/2)	25241	399	436	-1766	1316	358
$7d_{5/2}^1$	(J=5/2)	27071	389	447	-1765	-514	447
$8p_{3/2}^1$	(J=3/2)	37194	326	392	-1937	-3797	257
$E120^{2+}$	(J=0)	88907	446	554	-1701	-739	417
$8s_{1/2}^2$	(J=0) $\rightarrow$						
$8s_{1/2}^1 8p_{1/2}^1$	(J=0)	15012	266	310	-2354	6960	-100
$8s_{1/2}^1 8p_{1/2}^1$	(J=1)	17064	251	295	-2341	4908	-171
$8s_{1/2}^1 7d_{3/2}^1$	(J=1)	22207	366	401	-1632	585	316
$8s_{1/2}^1 7d_{3/2}^1$	(J=2)	22259	387	428	-1620	533	483
$8s_{1/2}^1 7d_{5/2}^1$	(J=3)	22968	386	436	-1617	-176	484
$8s_{1/2}^1 8p_{3/2}^1$	(J=2)	25009	253	297	-1842	-3037	384
$8s_{1/2}^1 7d_{5/2}^1$	(J=2)	27271	344	394	-1813	-262	291
$8s_{1/2}^1 8p_{3/2}^1$	(J=1)	27834	307	351	-1820	-1171	563
$8s_{1/2}^1$	(J=1/2)	47120	333	385	-1661	-687	381

To compare with the E120 transition energies, the corresponding experimental data for Ba from Ref. [17] are listed in table III. One can see that the barium excitation energies are smaller in general. It also indicates that E120 will possibly be more inert in general than Ba.

### Molecular calculations

In two-component molecular relativistic calculations and high-level correlation treatment only relatively small

TABLE III: The experimental transition energies (TE) from Ref. [17] for the lowest-lying states of the Ba atom and its cations. All values are in  $\text{cm}^{-1}$ .

Leading conf.	Term	Exper. TE Ref. [17]
$6s_{1/2}$	(J=1/2)	$\rightarrow$
$5d_{3/2}$	(J=3/2)	4874
$5d_{5/2}$	(J=5/2)	5675
$6p_{1/2}$	(J=1/2)	20262
$6p_{3/2}$	(J=3/2)	21952
$Ba^{2+}$	(J=0)	80686
$6s_{1/2}^2$	(J=0)	$\rightarrow$
$6s_{1/2}5d_{3/2}^1$	(J=1)	9034
$6s_{1/2}5d_{3/2}^1 + 6s_{1/2}5d_{5/2}^1$	(J=2)	9216
$6s_{1/2}5d_{5/2}^1$	(J=3)	9597
$6s_{1/2}5d_{5/2}^1 + 6s_{1/2}5d_{3/2}^1$	(J=2)	11395
$6s_{1/2}6p_{1/2}$	(J=0)	12266
$6s_{1/2}6p_{1/2} + 6s_{1/2}6p_{3/2}$	(J=1)	12637
$6s_{1/2}6p_{3/2}$	(J=2)	13515
$6s_{1/2}6p_{3/2} + 6s_{1/2}6p_{1/2}$	(J=1)	18060
$6s_{1/2}$	(J=1/2)	42035

basis sets can be used for diatomics like E120Au. At the same time, rather large basis sets can be employed in scalar-relativistic calculations of diatomic molecules. Therefore, the following scheme for the basis set generation was used in this work: (i) For each atom (E120, Ba and Au), a large set of primitive Gaussian functions capable of describing wave-functions of the ground and excited states of the corresponding atoms was generated. These basis sets will be referred as LBas below. LBas(E120) and LBas(Ba) consist of  $15s$ -,  $15p$ -,  $8d$ -,  $8f$ -,  $6g$ -,  $6h$ -type functions, which shortly can be written as  $[15,15,8,8,6,6]$ . (ii) Then scalar relativistic CCSD calculation is performed with the large basis set for an atom and its compound (E120, E120-H, E120-Au, etc.). (iii) Generation of a compact basis set of contracted Gaussian functions was performed in a manner similar to that employed for generating atomic natural basis sets [18]: the atomic blocks from the density matrix calculated at stage (ii) were diagonalized to yield atomic natural-like basis set. The functions with the largest occupation numbers were selected from these natural basis functions. The results obtained with the given basis set approximately reproduce those with the large basis set. Besides, the functions required for accurate reproducing the essentially different radial parts of the  $7p_{1/2}$  and  $7p_{3/2}$  spinors, as well as the  $8p_{1/2}$ ,  $8p_{3/2}$ ,  $7d_{3/2}$ , and  $7d_{5/2}$  spinors, have also been included to the new bases. These compact basis sets will be referred as CBas.

Finally, the following scheme to evaluate ionization potentials and dissociation energies of molecules was employed: (i) Calculation using two-component Fock-Space coupled cluster method with single and double ampli-

tudes in the CBas basis set. (ii) Calculation of corrections on enlargement of the basis set and contribution of triple cluster amplitudes by the scalar-relativistic coupled cluster method with single, double and non-iterative triple cluster amplitudes, CCSD(T), using LBas. (iii) Calculation of corrections on higher (iterative triple and non-iterative quadruple) cluster amplitudes by the scalar-relativistic coupled cluster method with single, double, triple and non-iterative quadruple cluster amplitudes, CCSDT(Q), using CBas.

Equilibrium internuclear distances in the considered diatomic molecules were calculated using the scalar-relativistic CCSD(T) method and LBas.

## RESULTS AND DISCUSSIONS

### Ionization potentials

Some properties of E120, of which the first (IP1) and second (IP2) ionization potentials are examples, are considered here in comparison with the corresponding properties of Ba. As was described above, the two-component FS-RCCSD method was used to calculate the main contributions to IP1 and IP2. These calculations were performed in compact basis sets, CBas, consisting of  $5s$ ,  $6p$ ,  $4d$ , and  $3f$  functions for E120 and of  $5s$ ,  $5p$ ,  $3d$ , and  $3f$  for Ba. The computed values for E120 are IP1= 47236  $\text{cm}^{-1}$  and IP2= 89061  $\text{cm}^{-1}$ , while for Ba IP1= 42340  $\text{cm}^{-1}$  and IP2= 80326  $\text{cm}^{-1}$ . Contributions from enlargement of the basis set up to  $15s$ ,  $15p$ ,  $8d$ ,  $8f$  and  $6h$  ( $[15,15,8,8,6,6]$ ) functions and non-iterative triple cluster amplitudes for E120 are -462  $\text{cm}^{-1}$  for IP1 and 31  $\text{cm}^{-1}$  for IP2 [25]. For Ba these values are -579  $\text{cm}^{-1}$  and -65  $\text{cm}^{-1}$ . Contributions of higher cluster amplitudes estimated using CCSDT(Q) method and  $[15,15,8,8,6]$  basis set ( $h$  functions were excluded) are negligible (less than 30  $\text{cm}^{-1}$ ). The final values of the ionization potentials for E120 and Ba are given in table VI together with the corresponding experimental values for Ba.

The theoretical uncertainty of the ionization potentials of E120 can be estimated from the corresponding atomic calculations (tables I and II) and is suggested to be within 1 kcal/mol  $\approx$  350  $\text{cm}^{-1}$ .

### X-H dissociation energies, X=E120, Ba

In order to estimate the stability of compounds of E120 compared to those of Ba we have first considered the dissociation energies of the corresponding hydrides since the experimental data are available for BaH [19]). Another often considered characteristic of SHE is the dissociation energy of its fluorides, X-F. However, the X-F bonding is not so illustrative qualitatively because almost all the elements (except light noble gases) are known to react in

a fluorine atmosphere yielding rather stable fluorides. At the same time the dimer systems such as Ba<sub>2</sub>, Hg<sub>2</sub>, Xe<sub>2</sub>, E112<sub>2</sub> are all the van der Waals systems with small dissociation energies. By contrast, the ground state of the XeH molecule is not observed in the gas phase, whereas BaH was obtained and characterized [20, 21].

To calculate E120H and BaH, the scheme similar to that for the calculation of the ionization potentials was used. Compact basis sets for E120, Ba and H were [5,6,4,2], [5,5,3,2] and [4,3,1], respectively. Large basis sets for E120 and Ba were [15,15,8,8,6], i.e. without *h*-functions. The aug-cc-pvqz [22] basis set was used as the large basis set for H. To exclude the basis set superposition errors, the diatomic molecules and atoms were calculated in the same two-center basis, i.e. the counterpoise corrections [23] were used.

The dissociation energy of E120H calculated within FS-RCCSD using the CBas(E120) and CBas(H) basis sets is 8258 cm<sup>-1</sup>, while the correction on the large basis and triple cluster amplitudes is -261 cm<sup>-1</sup>. For BaH the former contribution is 17061 cm<sup>-1</sup>, while the correction gives -430 cm<sup>-1</sup>.

The calculated spectroscopic properties of the BaH molecule are in a good agreement with the experimental data (see table IV).

TABLE IV: Calculated and experimental harmonic frequency ( $w_e$ ), vibrational anharmonicity ( $w_e x_e$ ), dissociation energy ( $D_0$ ) and equilibrium distance ( $R_e$ ) of the <sup>137</sup>BaH molecule,

	Calculation	Experiment
$w_e$ , cm <sup>-1</sup>	1158	1168 [20]
$w_e x_e$ , cm <sup>-1</sup>	14.1	14.5 [20]
$D_0$ , cm <sup>-1</sup>	16053	15728 [19]
$R_e$ , Å	2.238	2.232 [20]

The final values for the dissociation energies,  $D_e$ , of E120H and BaH are given in table VI. The equilibrium internuclear distance in BaH is on 0.2 Å shorter than that in E120H.

The theoretical uncertainty of the dissociation energy of E120H is estimated to be 500 cm<sup>-1</sup>.

It follows from table VI that the E120-H bond is significantly weaker than that in BaH. Partly it can be explained by the presence of lower-lying excited states in the case of Ba and its cation (see table III). Contribution of these states to the BaH chemical bond leads to its additional stabilization. In turn, the excited states in the case of E120 are lying significantly higher (see table II);

To check this viewpoint two series of scalar-relativistic calculations of the BaH and E120H dissociation energies were performed: (i) with *d*- and *f*-type basis functions in basis set (CBas); (ii) without *d* and *f* functions. The latter calculation prevents participating the *d* orbitals of Ba and E120 in chemical bonding of their hydrides. Note, however, that it is just test calculation because exclusion of *d* basis functions also prevents, e.g., correlation of

5*p*-electrons of Ba and 7*p*-electrons of E120 into these states. The results are given in table V.

TABLE V: Calculated dissociation energy of BaH and E120H using scalar-relativistic Hartree-Fock (HF) of CCSD(T) levels of theory in CBas basis set and CBas with excluded *d*-, *f*-functions (CBasNoD)

Basis	CBas		CBasNoD	
Method	HF	CCSD(T)	HF	CCSD(T)
$D_e$ (BaH), cm <sup>-1</sup>	13605	15957	7877	10677
$D_e$ (E120H), cm <sup>-1</sup>	2864	6865	-68	5264

It follows from table V that *d* functions (and higher harmonics) significantly contribute to bonding of the monohydrides under consideration. At the CCSD(T) level of theory, this contribution is 5280 cm<sup>-1</sup> to the Ba-H bond, while is only 1601 cm<sup>-1</sup> in E120H. These values confirm the qualitative discussion above based on the atomic transitions. However, even without *d* basis functions the BaH bond energy at the CCSD(T) level is twice stronger than that in E120H. This observation is in a qualitative agreement with the fact that the states with the valence *sp* (*p*) configurations in E120 (E120<sup>+</sup>) lies higher than the corresponding states in Ba (Ba<sup>+</sup>). It should be noted that the bonding in E120H is in essence due to the correlation effects when the CBasNoD basis set is used.

#### X-Au dissociation energies, X=E120, Ba

As the first stage of modelling interaction of E120 element with gold surface, the simplest comparative model, E120Au vs. BaAu, is considered here.

The 19-electron GRECP was used for Au. Thus, 29 electrons were treated in the correlation calculation. For E120Au, the relativistic two-component FS-RCCSD calculation in the Au[7,7,4,2] and E120[5,5,2,1] basis sets gives the dissociation energy of 11732 cm<sup>-1</sup>. Correction on the larger basis set ([15,15,8,8,7] for Au and [15,15,8,4] for E120) is 510 cm<sup>-1</sup>, contribution of non-iterative triple cluster amplitudes [25] is 2264 cm<sup>-1</sup> and correction on higher amplitudes (calculated as the difference between CCSDT(Q) and CCSD(T) energies in the compact Au[6,6,4,2,1] and E120[6,5,2,1] basis sets) is less than 100 cm<sup>-1</sup>. Similar calculations were performed for BaAu. The final calculated values are given in table VI. The equilibrium distance for BaAu is on 0.1 Å shorter than that in E120Au.

The theoretical uncertainty of the dissociation energy of E120Au is estimated to be 1000 cm<sup>-1</sup>.

TABLE VI: Calculated properties of E120 in comparison with Ba: the first and second ionization potentials (IP1 and IP2), dissociation energies ( $D_e$ ) of hydrides and aurides (X-Au) and the corresponding equilibrium distances ( $R_e$ ).

	E120-calc	Ba-calc	Ba-exp
IP1, $\text{cm}^{-1}$	47046	41932	42035 [24]
IP2, $\text{cm}^{-1}$	89286	80442	80686 [24]
$D_e(\text{X-H})$ , $\text{cm}^{-1}$	7997	16632	16308[19]
$R_e(\text{X-H})$ , Å	2.45	2.24	2.23 [20]
$D_e(\text{X-Au})$ , $\text{cm}^{-1}$	14428	22608	-
$R_e(\text{X-Au})$ , Å	3.1	3.0	-

## Conclusion

Properties of E120 and its compounds are considered in comparison with their Ba analogues. The monohydride and monoauride of E120 are found to be less stable than the corresponding analogues of the Ba compounds. Nevertheless, E120 can be rather considered as a “typical” representative of the second group.

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\* Electronic address: leonidos239@gmail.com

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- [25] We have also included here the corrections arising when going from the Fock-Space coupled clusters to the single-reference coupled clusters.